*Special Cases* :

(i) If we let $k \to 0$ in eq. (3) the solution given by eq. (4) reduces to the result of Goyal & Mathur [(1974)].

(ii) If we let $h \to 0$ in (2) the equation given by (4) yields us the result given by Gupta & Mathur [(1974)].

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# Group velocity of wave packets : A general formula

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The idea of wavepackets is of great utility for quantum-mechanical studies During the initial stages of the development of quantum-mechanics around 1925, the concept was used to explore the implications of uncertainty principle. For this objective, the wave functions were taken to be pure plane waves, i e., aves of the form : $\exp i\left[k r - \frac{E(k)}{\hbar} t\right]$ These investigations were thus concerned with the motion of free particles with non-relativistic energies and became important textural materials many decades ago (Schiff 1949; Messiah 1961). Sometime later, the idea of wave-packets was applied, quite interestingly, to the study of free particles with relativistic energies and a survey of the works in this direction can be found in the paper by Bakke & Wergeland (1974).

Although the application of the idea of wavepackets to the motion of free particles helped to elucidate considerably, as just mentioned, certain fundamental aspects of quantum mechanics, there occurred gradually the need for applying the concept to the study of particles which are moving under the action of certain

forces; situations like those are often met with in practice, a typical example being the motion of Bloch electrons in crystals. Now, while dealing with the notion of wavepackets, we come across the entity called the group velocity And it is this entity which provides the vital informations, obtainable on the basis of wave-packet formalism. Thus, to be able to use the idea of wave packets for the study of a physical system moving under forces, we need a formula for the group velocity of wave packets which are constructed out of such waves as accommodate the effect of the forces on the system An approach of this sort, though very necessary for treating many realistic systems, does not seem to have received any attention so far.

In the present communication, we have reported a general formula for the group velocity of wave packets, the constituents of which are chosen in keeping with the above considerations and in such a way as lucidly indicates their correspondence with the wave function for realistic system like Bloch electrons in crystal. While the commonly used formula [given by eq (25) is space-independent, the formula derived here is seen to be space-dependent The conditions under which the present formula would reduce to the usual space-independent form, are discussed

To begin with the derivation, we take the constituent members of the wave packets to be of the following form :

$$\phi_{\boldsymbol{k}}(r, t) = U(\boldsymbol{k}, r)\exp i\left[\boldsymbol{k}\, r - \frac{E(\boldsymbol{k})}{\hbar}\, t\right] \qquad \ldots \quad (1)$$

In eq (1), $E(\boldsymbol{k})$ is the energy momentum relation and $U(\boldsymbol{k}, r)$ is an amplitude term, dependent on both the ware vector $\boldsymbol{k}$ [with components $k_1$, $k_2$, $k_3$] and positional coordinate $r$ This amplitude term, $U(\boldsymbol{k}, r)$, takes care of the effect of the force under which the system moves. Now a packet $\psi(r, t)$, of waves given by eq (1), appears as

$$\psi(r, t) = \int A(\boldsymbol{k}) U(\boldsymbol{k}, r)\exp i\left[\boldsymbol{k}.r - \frac{E(\boldsymbol{k})}{\hbar} t\right] d^3k \qquad \ldots \quad (2)$$

In (2), the modulus $|A(k)|$ of $A(k)$ is assumed to have a sharp maximum at $k = k_0$, i.e , at $(k_1, k_2, k_3) = [(k_0)_1, (k_0)_2, (k_0)_3]$ and falls fast to zero on either side of $(k_0)_1$, $(k_0)_2$ and $(k_0)_3$ The range of integration in eq (2) is the region in which $|A(k)|$ is appreciably different from zero. In constructing a wave packet in the form eq. (2), we make no other assumptions than those about $A(k)$, hence, all the results extracted out of the wave packet (2) would be general, in the sense that they would not be dependent on any approximation regarding the variation of $U(\boldsymbol{k}, r)$ with respect to $\boldsymbol{k}$ or $\boldsymbol{r}$.

Now we can write (2) in the following form :

$$\psi(r, t) = \int |A(\boldsymbol{k})| \, |U(\boldsymbol{k}\ r) \exp i\,[\theta\,(\boldsymbol{k}, r, t)] d^3k \qquad \ldots \quad (3)$$

where,

$$\theta(\boldsymbol{k}, r, t) = k.r - \frac{E(\boldsymbol{k})}{\hbar} t + \alpha(\boldsymbol{k}) r) + \beta(\boldsymbol{k}, r) \qquad \ldots \quad (4)$$

$$\alpha(k, r) = \text{the phase angle of } U(\boldsymbol{k}, r) = \tan^{-1} \frac{U_1}{U_2} \qquad \ldots \quad (5)$$

$$U(\boldsymbol{k}, r) = U_1(\boldsymbol{k}, r) + iU_2(\boldsymbol{k}, r) \qquad \ldots \quad (6)$$

$$\beta(\boldsymbol{k}) = \text{the phase angle of } A(\boldsymbol{k}) = \tan^{-1} \frac{A_1(\boldsymbol{k})}{A_2(\boldsymbol{k})} \qquad \ldots \quad (7)$$

$$A(\boldsymbol{k}) = A_1(\boldsymbol{k}) + iA_2(\boldsymbol{k}): \qquad \ldots \quad (8)$$

In order that eq. (3) may give a non vanishing value for $\psi(r, t)$, $\theta(\boldsymbol{k}, r, t)$, for the given space-time point $(r, t)$ must remain constant with respect $\boldsymbol{k}$-values lying within the range of integration. This condition, in turn leads to the following relations .

$$\frac{\partial\theta}{\partial k_1} = \frac{\partial\theta}{\partial k_2} = \frac{\partial\theta}{\partial k_3} = 0. \qquad \ldots \quad (9)$$

With the help of eqs. (4)—(9), we get the following results

$$\frac{\partial\theta}{\partial k_1} = x - \left(\frac{\partial E}{\partial k_1}\right) t/\hbar + \frac{\partial\alpha}{\partial k_1} + \frac{\partial\beta}{\partial k_1} = 0 \qquad \ldots \quad (10)$$

$$\frac{\partial\theta}{\partial k_2} = y - \left(\frac{\partial E}{\partial k_2}\right) t/\hbar + \frac{\partial\alpha}{\partial k_2} + \frac{\partial\beta}{\partial k_2} = 0 \qquad \ldots \quad (11)$$

$$\frac{\partial\theta}{\partial k_3} = z - \left(\frac{\partial E}{\partial k_3}\right) t/\hbar + \frac{\partial\alpha}{\partial k_3} + \frac{\partial\beta}{\partial k_3} = 0 \qquad \ldots \quad (12)$$

From eqs. (10), (11) and (12), the components $dx/dt( = v_1)$, $dy/dt(= v_2)$ and $dz/dt\,(= v_3)$, of the group velocity are obtained as solution of the following matrix equation

$$M \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} \qquad \ldots \quad (13)$$

where,

$$c_i = \frac{1}{\hbar}\left(\frac{\partial E}{\partial k_i}\right) ; \; i = 1, 2, 3; \qquad \ldots \quad (14)$$

The matrix $M$ is given by :

$$M = \begin{pmatrix} \{1+\alpha_{x1}\} & \alpha_{y1} & \alpha_{z1} \\ \alpha_{x2} & \{1+\alpha_{y2}\} & \alpha_{z2} \\ \alpha_{x3} & \alpha_{y3} & \{1+\alpha_{y3}\} \end{pmatrix} \quad \ldots (15)$$

$$\alpha_{qj} = \frac{\partial}{\partial q_j} \frac{\partial \alpha}{\partial q} \left( \frac{\partial \alpha}{\partial k_j} \right), \quad q = x, y, z; \quad j = 1, 2, 3.$$

By solving eq (13), we get $v_i$'s explicitly as .

$$v_1 = \frac{1}{1+\alpha_{x1}} \left[ c_1 - \alpha_{y1} \frac{\gamma_2\beta_1 - \delta_2\beta_2}{\gamma_2\delta_1 - \delta_2\gamma_1} - \alpha_{z1} \frac{\gamma_1\beta_1 - \delta_1\beta_2}{\gamma_1\delta_2 - \delta_1\gamma_2} \right] \quad \ldots (16)$$

$$v_2 = \frac{\gamma_2\beta_1 - \delta_2\beta_2}{\gamma_2\delta_1 - \gamma_1\delta_2} \quad \ldots (17)$$

$$v_3 = \frac{\gamma_1\beta_1 - \delta_1\beta_2}{\gamma_1\delta_2 - \delta_1\gamma_2} \quad \ldots (18)$$

$\beta_1, \beta_2 \ldots$ etc. are given below .

$$\beta_1 = c_1\alpha_{x2} - (1+\alpha_{x1})c_2 \quad \ldots (19)$$

$$\beta_2 = c_1\alpha_{x3} - (1+\alpha_{x1})c_3 \quad \ldots (20)$$

$$\gamma_1 = \alpha_{y1}\alpha_{x3} - (1+\alpha_{x1})\alpha_{y3} \quad \ldots (21)$$

$$\gamma_2 = \alpha_{z1}\alpha_{x3} - (1-\alpha_{x1})(1+\alpha_{z3}) \quad \ldots (22)$$

$$\delta_1 = \alpha_{x2}\alpha_{y1} - (1+\alpha_{x1})(1+\alpha_{y2}) \quad \ldots (23)$$

$$\delta_2 = \alpha_{a3}(1+\alpha_{z3}) - (1+\alpha_{x1})(1+P_{z3}) \quad \ldots (24)$$

The formulae (16)–(18), for the components of the group velocity, are seen to be dependent on $\boldsymbol{k}$ as well as the space coordinates $\boldsymbol{r}$ of the moving system, the latter dependence coming through $p(k, r)$. The group velocity normally reported in literature is, on the other hand, dependent only on the momentum $\boldsymbol{k}$ and appears explicitly as

$$\boldsymbol{v} = \frac{1}{\hbar} \nabla_{\boldsymbol{k}}[E(\boldsymbol{k})] \quad \ldots (25)$$

The space-dependence of our formulae is thus an entirely new feature. It can be noticed easily that our results reduce to eq. (25) when the space-variation of $\boldsymbol{\alpha}$ can be ignored; this condition means in turn, on account of eq. (5), that our results would reduce to eq. (25) when the space-variation of $U(\boldsymbol{k}, r)$ can be neglected.

As mentioned earlier, the amplitude function $U(k, r)$ incorporates in the wavefunction the characteristics of the forces under which the system moves. What we have tried to show here is the general effect of the presence of the function $U(k, r)$, (hence, of the forces acting on the system) upon the group velocity We wish to discuss in a future communication the application of the formulae (16)–(18), to Bloch electrons moving in crystalline solids for which the $U$ function satisfies the well known condition : $U(\boldsymbol{k}, r) = U(\boldsymbol{k}, r + R_j)$ where $R_j$'s are the lattice vectors

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# The crystal structure of 3-5 di-methoxy homophthalic acid $C_{11}$ $H_{12}$ $O_6$

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The investigation of this compound was undertaken to establish the molecular geometry and the scheme of hydrogen bonding in the crystal.

*Crystal data*

Triclinic with $a = 8.01$, $b = 13.90$, $c = 5.23$Å, $\alpha = 105.6°$, $\beta = 80\,5°$ and $\gamma = 104.2°$. $D_{calc} = 1\,47$, $D_{obs} = 1\,48$ gm cm$^{-3}$, $Z = 2$. space group $P_1$.

*Structure determination*

720 reflexions were collected from single crystal Weissenberg photography using CuK unfiltered radiation. The structure was solved using the programme MULTAN (Germain, Main & Woolfson 1971) and in the present stage of least-squares refinement $R(hkl)$ for the observed reflexions is 18·1%.

*Comments*

A view of the crystal structure looking from [001] is shown in figure 1. In the crystal, the molecules form dimers through their two carboxyl groups, which are linked across centres of symmetry, the hydrogen bonds being 2·73 and 2·81 Å.